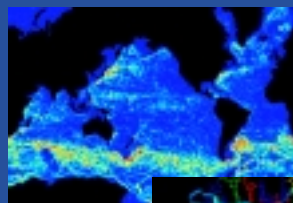


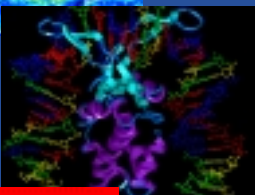


Office of Science

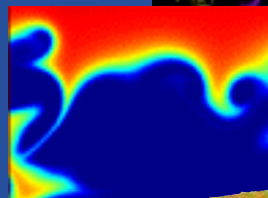
U.S. Department of Energy



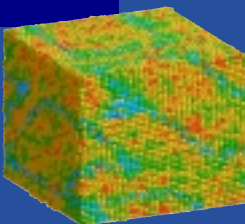
*Global  
Change*



*Proteins*



*Combustion  
Chemistry*



*Materials  
Science*

# Advanced Scientific Computing Research

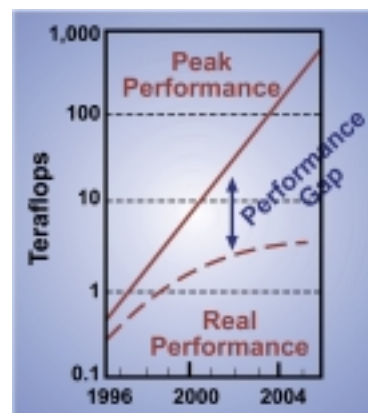
The Office of Science's Advanced Scientific Computing Research (ASCR) program supports fundamental research in advanced scientific computing—applied mathematics, computer science, and networking—and provides world-class, high-performance computational and networking tools that enable the Department of Energy (DOE) to succeed in its science, energy, environmental quality, and national security missions. In 2001, the program funded research at 65 academic institutions and 10 DOE laboratories. More than 2,400 scientists in universities, Federal agencies, and U.S. companies use ASCR-funded high-performance computers. Research communities that benefit from these resources include structural biology; superconductor technology; medical research and technology development; materials, chemical, and plasma sciences; high energy and nuclear physics; and environmental and atmospheric research.

## The Opportunity

Computational modeling and simulation made dramatic contributions to the advancement of science in the 20<sup>th</sup> Century. Driven by rapid technological advances within the past two decades, computing and high-speed networking have emerged as powerful tools for science. However, unless software keeps pace with the terascale computers being developed, scientists will not be able to take full advantage of these powerful new research tools. A focus for ASCR is to bring software advances up to the same level as these hardware advances. These computational tools are essential to the development of new energy technologies and the discovery of new scientific knowledge. The Office of Science has numerous scientific questions that can only be addressed through advances in scientific computing, such as predicting climate change or understanding complex biological systems.

## The Challenge

Current advances in computing technology are being driven by market forces in the commercial sector, not by the need to solve scientific questions. ASCR works to close this gap by developing the software needed to harness commercial computing technology for scientific research problems of a magnitude and complexity never before addressed through computational modeling. ASCR's research will focus on the following areas:



**Mathematical Microscopy.** DOE's mission requires an understanding of the role of microorganisms in climate change and energy production, the bio-remediation of energy and nuclear materials waste, the health risks of low-dose radiation exposure, and the basic bioscience needed for effectively defending against biological attack. ASCR contributes to this mission by developing the mathematical tools that will provide insight and prediction of the complex and evolving behavior of the "molecular machines of life." Specifically, ASCR is focused on the development of new mathematical methods that will enable breakthrough advances in computational techniques for solving complex biological problems.

### Taming Computational Complexity.

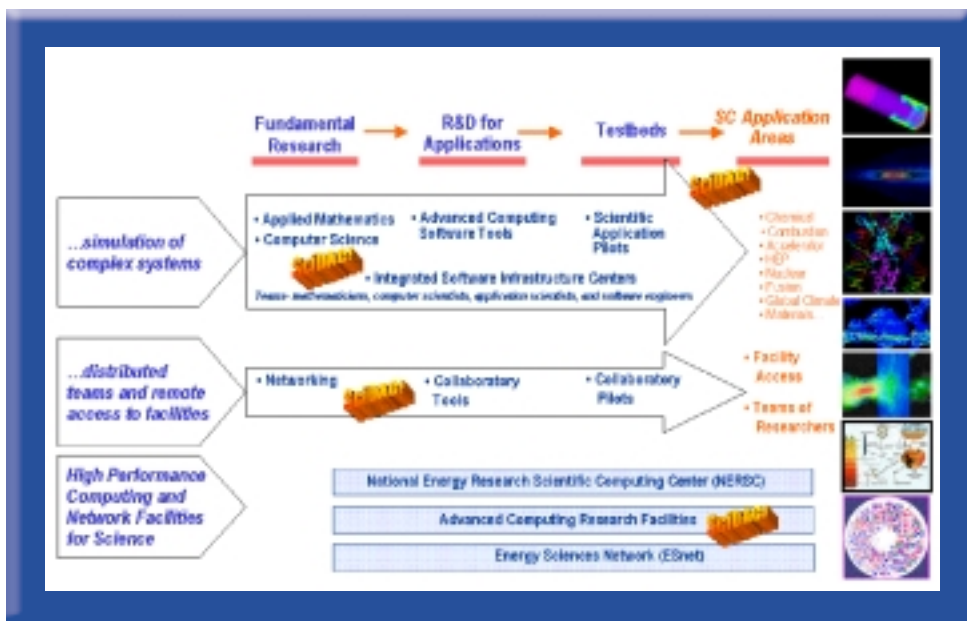
ASCR is working to create the software environments that will enable petascale computation to solve DOE's breakthrough scientific problems. Such problems are large, highly complex, multidisciplinary, and span a wide range of both space and time scales. Computer science research provides the software environments that enable scientists to conduct computational experiments and analyses quickly and easily, fostering comprehension of new phenomena and thus enabling scientific discovery.

**Collaboratories/Software Tools.** ASCR is developing systems to enable scientists to remotely access and control facilities and share data effectively with colleagues on a routine basis. Advanced networking and distributed computing techniques must become ubiquitous. Existing barriers associated with remote resource access and the integration of geographically distributed resources must be overcome through the development of innovative software tools and protocols.

## Investment Plan

ASCR will strengthen its commitment to high-performance scientific computing by developing a new generation of scientific simulation codes that take full advantage of the extraordinary computing capabilities of terascale computers. The ASCR program will also develop high-performance computers designed for a specific suite of applications, known as

Topical Computing Centers. These Centers will be provided to research teams developing new generations of large computational models. ASCR research activities in mathematics, computer science, and specialized software tools will be enhanced to support the develop-



*Computing systems hardware and software infrastructure*

ment of science-based simulations of multi-protein molecular machines, as well as structures and interactions at the nanoscale.

## The Benefits

High-performance computing provides a new window for researchers to observe the natural world at a fidelity that could only be imagined a few years ago. Research investments in advanced scientific computing equip researchers with premier computational tools to advance knowledge and to solve the most challenging scientific problems facing the Nation.

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